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DIRECT SOLUTION OF LANDAU-LIFSHITZ-GILBERT EQUATION FOR DOMAIN WALLS IN THIN PERMALLOY FILMS

Nobuo Hayashi, Toshiaki Inoue, Yoshinobu Nakatani
University of Electro-Communications, 1-5-1 Chofugaoka, Chofu-shi, Tokyo 182, Japan

Hiroshi Fukushima
Mobara Works, Hitachi, Ltd., 3300 Hayano, Mobara-shi, Chiba 297, Japan

The Gilbert equation expressed in conventional polar angle notation is solved for one-dimensional Neel and Bloch walls in a thin Permalloy film using different numerical methods to compare the extent of stability. The methods examined include the Euler, so-called modified Dufort-Frankel and backward Euler methods. The backward Euler method is found to be stable under arbitrary magnitude of time difference for the case of Neel walls if the contribution of the magnetization of the nearest-neighboring cells to the demagnetizing field was treated implicitly. The method is also stable in the case of Bloch walls, though the stability limit for the time step was only 10 times as large as that of the Euler method. The Dufort-Frankel method is found quite unstable. Two-dimensional computation is found feasible using the backward Euler method. The principle and the results of the calculations are given.

Introduction

While computation of wall structures in Permalloy films was mostly carried out based on variational method [1]-[4], direct solution of the Gilbert equation was reported in abundance for domain walls in bubble materials. Because of the large magnetization of Permalloy, however, the equation includes drastically increased demagnetizing torques, which may affect the stability of the numerical solution. It is the purpose of the present paper to examine whether or not the methods of discretizing the Gilbert equation which are useful in the case of bubble material are also useful in the case of Permalloy.

One-dimensional Neel and Bloch wall structures are calculated using the Euler [6], so-called modified Dufort-Frankel [5], [6] and backward Euler [6] methods for that purpose. To examine the feasibility of large-scale computation, planar two-dimension wall structures are also calculated using the backward Euler method.

Definition of the problem

We solve the Gilbert equation expressed in the polar and azimuthal angles, θ and ϕ , of the magnetization vector \vec{M} as in [6] and [7]:

$$(M/\gamma)(\alpha\dot{\theta} - \dot{\phi}\sin\theta) = \delta\epsilon/\delta\theta = f(\theta, \phi),$$

$$(M/\gamma)(\dot{\theta} + \alpha\dot{\phi}\sin\theta) = (1/\sin\theta)\delta\epsilon/\delta\phi = g(\theta, \phi),$$

denoting with ϵ the magnetic energy density of the system.

The polar (z) axis must be chosen in such a way that θ never approaches zero (mod π) as described in [6] and [7]. Thus different coordinates systems are used to calculate Neel and Bloch structures (Fig. 1). While the main frame to be used for the Neel walls has the z -axis in the film normal, the Z -axis is in the film plane and perpendicular to the wall tangent in the subsidiary frame to be used for the Bloch walls. Using the main frame, for example, the magnetic energy density can be expressed as

$$\epsilon(\theta, \phi) = A[(\nabla\theta)^2 + \sin^2\theta(\nabla\phi)^2] - K\sin^2\theta\sin^2\phi - \vec{M} \cdot \vec{H}/2$$

denoting the self-demagnetizing field by H .

In the one-dimensional calculations we consider a Permalloy film of thickness h and width xw (or Zw) as shown in Fig. 1. We divide the film along the x (or Z) axis into N_x (or N_z) prisms of equal size which extend in the y (or Y) direction. The free boundary condition is used at the film edges.

In the two-dimensional calculations a rectangular film is divided into N_x by N_y cells of equal size as shown in Fig. 2. The easy axis is taken parallel to y - or J -axis. Using an initially defined angle parameter S , the coordinates frame is selected at each cell (I, J) as follows: if the polar angle measured from the film normal is between $\pi - S$ and S at cells (I, J) and ($I \pm 1, J \pm 1$), the main frame

is selected. Otherwise the subsidiary frame is selected. In Fig. 2 the subsidiary frame is used around the film center because of the existence of a Bloch line of "circulation" type. The parameter S is chosen between 10 and 80 degrees, depending on the mesh size used. The free boundary condition is used at all film edges.

Because the purpose of the present paper is to compare the capability of different numerical methods, we make the following simplifications: 1) The Gilbert damping parameter is chosen arbitrary. 2) Possible eddy current effects are not considered. 3) The magnetization is not allowed to vary through the thickness of the film.

Numerical methods

The numerical methods used to examine the one-dimensional calculation can be summarized as follows. In the Euler method the time derivatives are replaced by the respective forward differences. In the finite difference form of the reversible torques f and g the first and the second-order spatial derivatives are evaluated at the

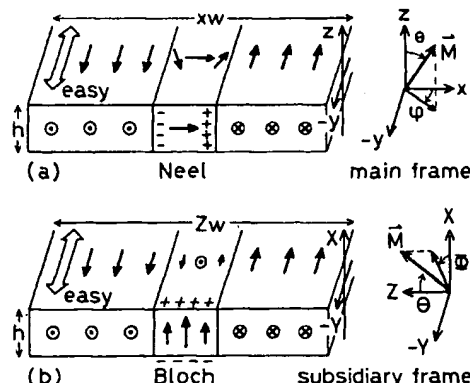


Fig. 1 Coordinates systems for (a) Neel and (b) Bloch walls.

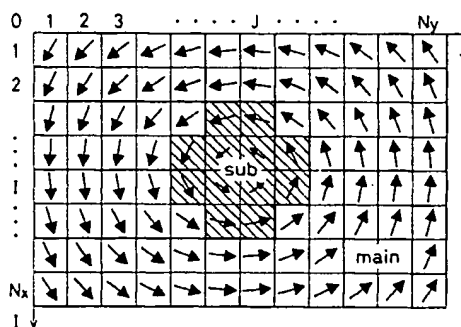


Fig. 2 Computing region and dual coordinates system for two-dimensional calculation. An equilibrium state derived from $h = 300$ Å, $\delta x = \delta y = 70$ Å, $N_x = 8$ and $N_y = 12$ is shown.

current time and discretized according to the midpoint formula. In the Dufort-Frankel method the time derivatives are discretized according to the midpoint formula. As to the spatial derivatives, a correction term is added to the midpoint difference evaluated at the current time. In the present paper the method modified according to [5] so as to increase the stability is used [6].

In the backward Euler method the time derivatives are replaced by the respective backward difference quotients with respect to time. The reference time is shifted to $t + \Delta t$, one step after the current time, t . The torque terms f and g are also evaluated at $t + \Delta t$, and expanded at time t so that terms of $O(\Delta t)$, $\Delta \theta$ and $\Delta \phi$ are retained. In the Newton's method the Euler equation associated to ϵ is solved, instead of the Gilbert equation, to obtain equilibrium configuration. The Euler equation discretized according to the Newton's iteration scheme is nothing but the Gilbert equation discretized according to the backward Euler method with time step Δt of infinity [6].

The spatial derivatives of exchange origin are replaced by the linear combinations of the values at the mesh points i under consideration and the two neighboring points $i \pm 1$. Thus we have a set of simultaneous linear equations in which $\Delta \theta$ and $\Delta \phi$ at mesh points i and $i \pm 1$ are coupled [6],[7].

The demagnetizing field H is calculated with a finite grid method [1] collecting all charges appearing on the surfaces of the cells within the computing region. Theoretically the backward Euler and the Newton's iteration schemes require to collect the contributions of $\Delta \theta$ and $\Delta \phi$ among all the mesh points in the computing region, which makes all the cells in the computing region coupled in the aforementioned simultaneous equations. As in [6] and [7], however, only the contribution of the cell under consideration and the neighboring cells is included in most of the present calculations so that we may not have simultaneous equations with a "dense" coefficient matrix. Thus it would be more proper to call the presently used methods "incomplete Newton's method" and "incom-

plete backward Euler method" because long-range magnetostatic couplings are neglected.

The actual calculation reveals that 1) Unlike the case with bubble material the Dufort-Frankel method is quite unstable; 2) The incomplete backward Euler method allows us to use a time step at least 10 times larger than the largest time step which can be used with the Euler method; and that 3) In the case of Neel walls Newton's iteration schemes, both original and incomplete, converge stably, which would mean that the backward Euler method is stable with arbitrary magnitude of Δt .

In the light of the results of one-dimension calculation the two-dimension calculation was performed using the incomplete backward Euler method only. The numerical techniques for two-dimension calculation such as the use of dual coordinates frame and implicit treatment of the demagnetizing field are the same as in [6] and [7] except for the use of the so-called ILUCGS method [8] in the solution of the simultaneous linear equations.

Results

We use as material parameters $M=800G$, $A=1.0 \times 10^{-6}$ erg/cm, $K=1000$ erg/cm³, $\gamma=1.76 \times 10^3$ rad/Oe·s and $\alpha=1.0$. The equilibrium states obtained from the one-dimensional calculation are shown in Fig. 3. The initial value for ϕ was chosen as

$$\begin{aligned} \phi(i) &= -\pi/2 + 0.3\pi(i/Nx), & i \leq Nx/2 \\ &= \pi/2 - 0.3\pi(Nx-i)/Nx, & i \geq Nx/2 \end{aligned}$$

in the case of Neel walls. A step-like Φ jumping from $-\pi/2$ to $\pi/2$ at the wall center was used in the case of Bloch walls. A constant polar angle of $\pi/2$ was used in both Neel and Bloch walls. The incomplete Newton's method was used in the case of Neel walls. The calculation was repeated about 150 times until the rms value of

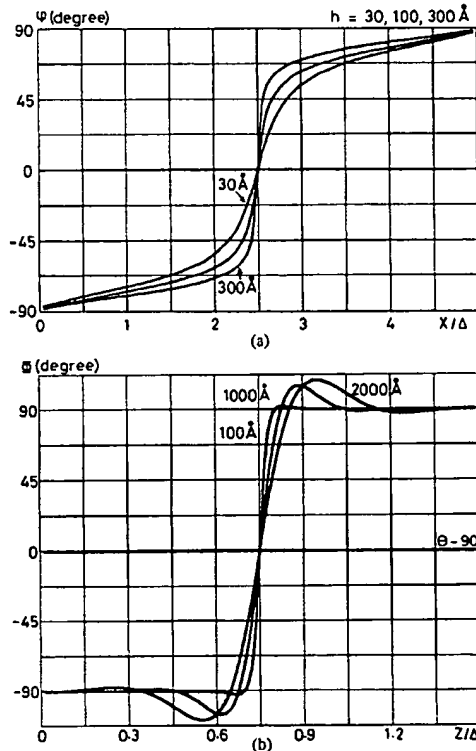


Fig.3 Neel (a) and Bloch (b) walls in equilibrium.

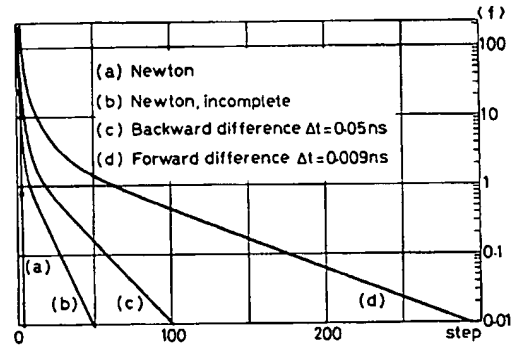


Fig.4 Average residual torque vs. calculation step derived from different methods. The case of Neel wall in a 100Å-thick film is shown.

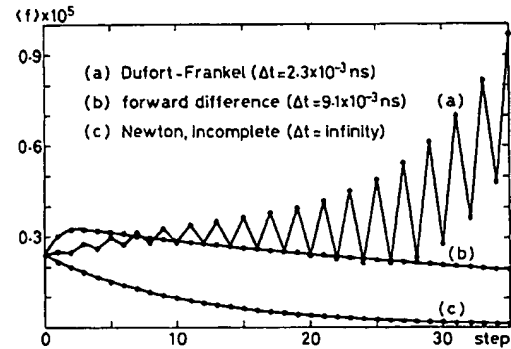


Fig.5 Comparison of numerical stability. The configuration derived from 140 iterations in the Newton's method (Fig.4) is used as the common initial state.

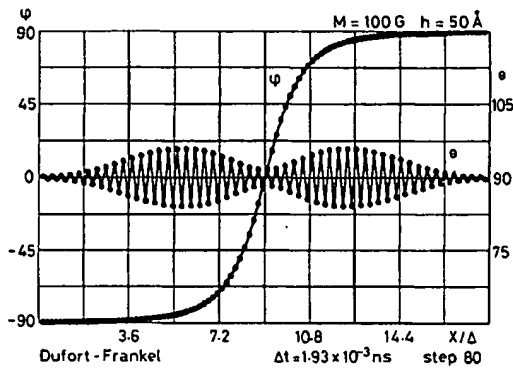


Fig. 6 Example of unstable calculation.

the residual reversible torque decreased to 10^{-6} of the initial value. The Bloch structures were calculated using the incomplete backward Euler method with $\Delta t \sim 0.02$ ns. The calculations were observed to converge after ~ 100 steps.

The speed of convergence observed in the calculation of the Neel wall using different methods is summarized in Fig. 4, where the Δt used is indicated. The figure shows that incomplete Newton's iteration converges much faster than the Euler, or forward difference, method. We know, however, that incomplete Newton's iteration converges almost in several steps in the case of one-dimensional charged and Bloch walls in bubble material. The difference in the convergence speed would be ascribed to the extremely large demagnetizing field in Permalloy films. Although not practical, it is interesting to note that the original Newton's method converges in a few steps even in the case of Permalloy. For one-dimension Bloch walls in Permalloy films, which are accompanied by much larger demagnetizing field, incomplete Newton's method was observed to diverge and the upper bound of Δt in the backward Euler method was only 10 times as large as that in the Euler method. The calculation using the original Newton's method was observed to converge even in that case.

The modified Dufort-Frankel method is attractive in that it leads to an explicit solution not requiring solving simultaneous equations. The method was more stable than the Euler method in the case of bubble material [6]. The method, however, was found quite unstable when applied to Permalloy films as shown in Figs. 5

and 6. When M is varied, the method was stable if $M < 100$ G. Figure 6 shows a transient Neel type configuration which appeared in the process of an unstable solution obtained with $M = 100$ G.

Figure 7 shows an example of planar two-dimensional calculation performed with the backward Euler method. The inplane component of M was given initially in a concentric configuration around the film center. The initial value of the film-normal component of M was given by

$$\theta(I, J) = 2 \arctan[\exp(4r(I, J)/l_B)] - \pi/2$$

with l_B and r denoting $\pi(A/2\pi M^2)^{1/2}$ and the distance of the mesh point (I, J) from the film center, respectively. The figure shows the configuration after 133 step calculation, where the rms value of the residual torque decreased to 5.4×10^{-7} of the initial value. The computation time was 10.75 minutes/step on a MELCOM-COSMO 800 with an operating speed of 1.2 million instructions/s. The required main memory space was 1.6 Mbytes.

Conclusion

One-dimensional wall structures in thin Permalloy films were calculated using the Gilbert equation discretized according to various numerical methods in order to compare the capability of each method to suppress the numerical instability. The results of the calculation show that the backward Euler method gives the largest time step which can be used without inducing instability and that the so-called modified Dufort-Frankel method cannot be used in the calculations for Permalloy films. The backward Euler method combined with ILUCGS method is also shown to be useful for medium to large scale two-dimension calculation. On closing the authors would like to thank Prof. Takao Suzuki of Tohoku University (presently with IBM Research Division, Almaden Research Center) for his valuable comments on the present work.

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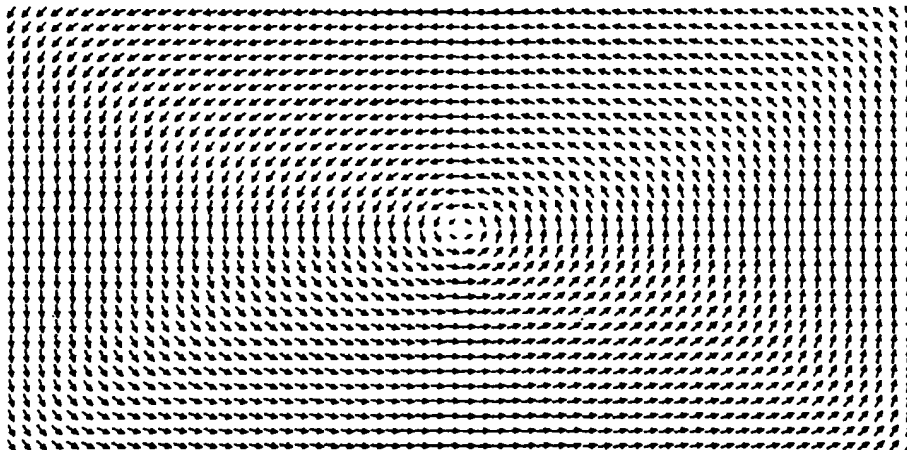


Fig. 7 Small closure-flux equilibrium configuration derived from 2D planar calculation. The parameters used are: $h=200$ Å, $\delta x=\delta y=50$ Å, $N_x=30$, $N_y=60$, $S=80^\circ$ and $\Delta t=0.01$ ns.